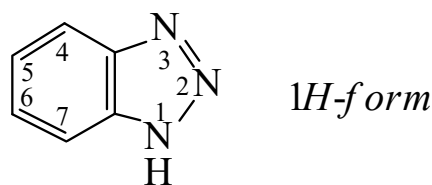




>>Entry Name: **Benzotriazole**

Synonym(s): Aziminobenzene (obsol.). 1,2,3-Triazaindene



CAS Registry Number: 95-14-7

Related CAS Registry Numbers(s): 273-02-9 22257-44-9

Molecular Formula: $C_6H_5N_3$

Molecular Weight: 119.126

Accurate Mass: 119.048347

Percentage Composition: C 60.50%; H 4.23%; N 35.27%

General Statement: 1*H*-Form predominates (>99.9%)

Use/Importance: Used for pptn. separation and gravimetric detn. of Ag, Cd, Co, Ni, Zn. The benzotriazolyl group is an extremely versatile substituent showing props. of leaving group, electron donor and ability to promote adjacent proton loss. Used in enamine synthesis

Physical Description: Needles (C_6H_6)

Melting Point: Mp 100°

Solubility: Sol. C_6H_6

pKa Value: pK_{a1} 1.6; pK_{a2} 8.64 (20°)

Hazard & Toxicity: Can detonate during vac. dist. Severe eye and skin irritant. LD₅₀ (rat, orl) 600 mg/kg

Aldrich: B1140-0

Fluka: 12799

Sigma: B1254

>>Variant: 1*H*-form

Molecular Formula: $C_6H_5N_3$

Molecular Weight: 119.126

Accurate Mass: 119.048347

Percentage Composition: C 60.50%; H 4.23%; N 35.27%

>>Derivative: *N*-Ac

CAS Registry Number: 18773-93-8

Molecular Formula: $C_8H_7N_3O$

Molecular Weight: 161.163

Accurate Mass: 161.058912

Percentage Composition: C 59.62%; H 4.38%; N 26.07%; O 9.93%

Melting Point: Mp 51°

>>Derivative: *N*-Benzoyl

CAS Registry Number: 4231-62-3

Molecular Formula: $C_{13}H_9N_3O$

Molecular Weight: 223.234

Accurate Mass: 223.074562

Percentage Composition: C 69.95%; H 4.06%; N 18.82%; O 7.17%

Melting Point: Mp 112°

>>Derivative: *N*-Chlorocarbonyl

Synonym(s): 1*H*-Benzotriazole-1-carbonyl chloride. 1-Chlorocarbonylbenzotriazole

CAS Registry Number: 65095-13-8

Molecular Formula: $C_7H_4ClN_3O$

Molecular Weight: 181.581

Accurate Mass: 181.004289

Percentage Composition: C 46.30%; H 2.22%; Cl 19.52%; N 23.14%; O 8.81%

Use/Importance: Synthetic reagent

Physical Description: Cryst. (petrol)

Melting Point: Mp 54-55°

>>Derivative: *N*-Hydroxy